National Aeronautics and
Space Administration

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

Retrieval of vertical *T*, H_2O, O_3, and CO_2 profiles, with sensitivity analysis (SA) and uncertainty quantification (UQ)

Paul Dimotakis, Luke Chen, Zhijin Li, Stephen Licata, Edward Olsen, and Thomas Pagano

Jet Propulsion Laboratory, California Institute of Technology

AIRS Science Team Meeting
24-27 April 2012, Caltech, Pasadena, CA

Objectives

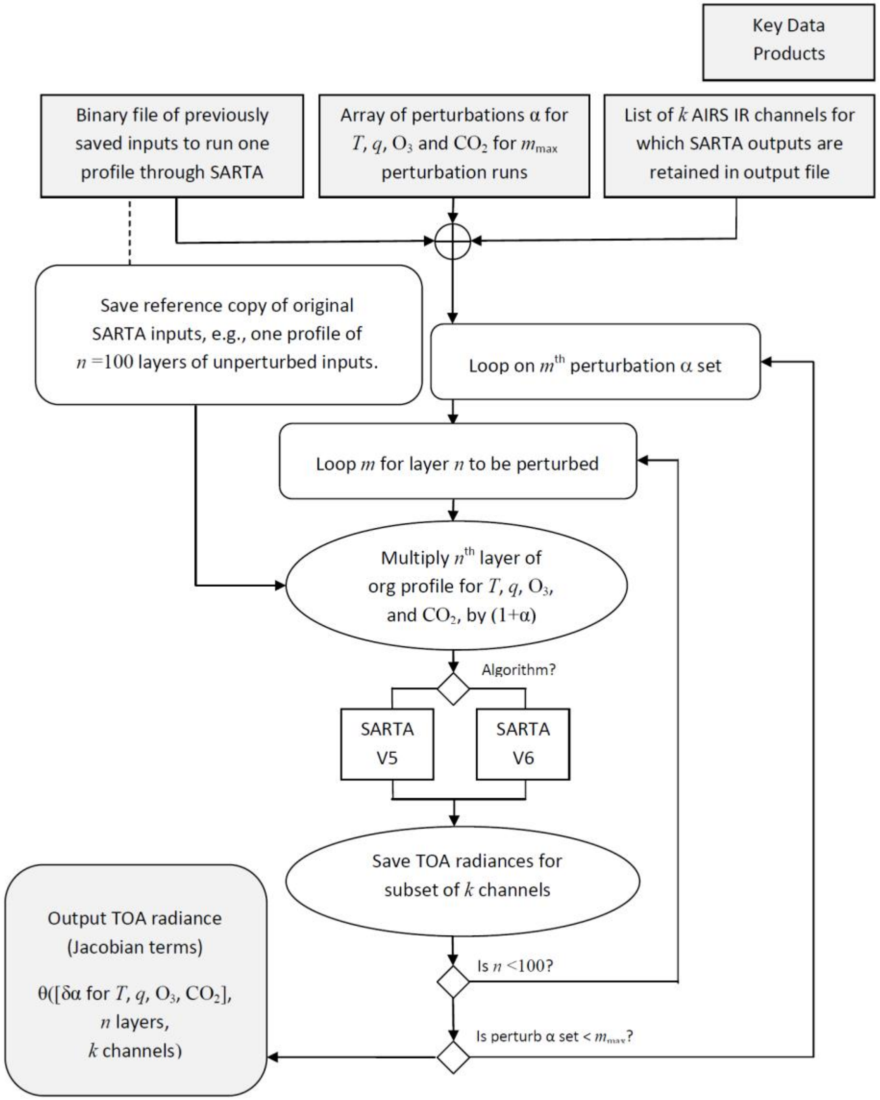
- **Augment retrieval methods for temperature (T), H_2O, O_3, and CO_2 to enable vertical-profile estimation for CO_2, with embedded sensitivity analysis (SA) and uncertainty quantification (UQ)**
  - **Adapt and evolve existing algorithmic methods and tools to support sensitivity analysis (SA) and uncertainty quantification (UQ)**
  - **Embed in analyses of maximum-likelihood estimation (MLE) retrievals to support and improve:**
    - **instrument calibration,**
    - **algorithm verification, and**
    - **data validation.**
- **Assess differences between retrieval approaches, e.g., "Optimal Estimation (OE)" and "Vanishing Partial Derivatives (VPD)", and map into a single unified scheme**
- **Characterize and quantify retrieval errors. Use results to:**
  - **identify dominant sensitivities to improve retrieval algorithms, and**
  - **assess and qualify data variances between retrievals and validation**
- **Explore application to vertical-profile estimations, extending to near-surface retrievals**

Approach

- **Formulation of sensitivity analysis (SA) and uncertainty quantification (UQ) framework and methods**
  - **Adopt maximum-likelihood estimation (MLE) methods**
  - **Develop concepts for Monte Carlo methods, DAKOTA,* linearity tests, …**
  - **Explore projection onto vertical-profile basis functions.**
- **Extend/adapt existing analysis tools, and develop new tools, as necessary, to support SA/UQ functionality**
  - **Tools that employ the Standalone AIRS Radiative-Transfer Algorithm (SARTA) for the analysis of channel selection and the calculation of retrieval Jacobians, in support of SA/UQ**
  - **Adapt contribution-function estimation for vertical-profile retrieval data**
- **Adapt observation-error analyses, based on maximum-likelihood estimation (MLE) methods**
  - **Link to analyses of frequency-calibration shifts.**
  - **Examine explicit and implicit assumptions in MLE estimations and compare “OE” and “VPD” approaches**
  - **Perform preliminary/idealized UQ analyses to explore and demonstrate UQ concepts and formulations.**

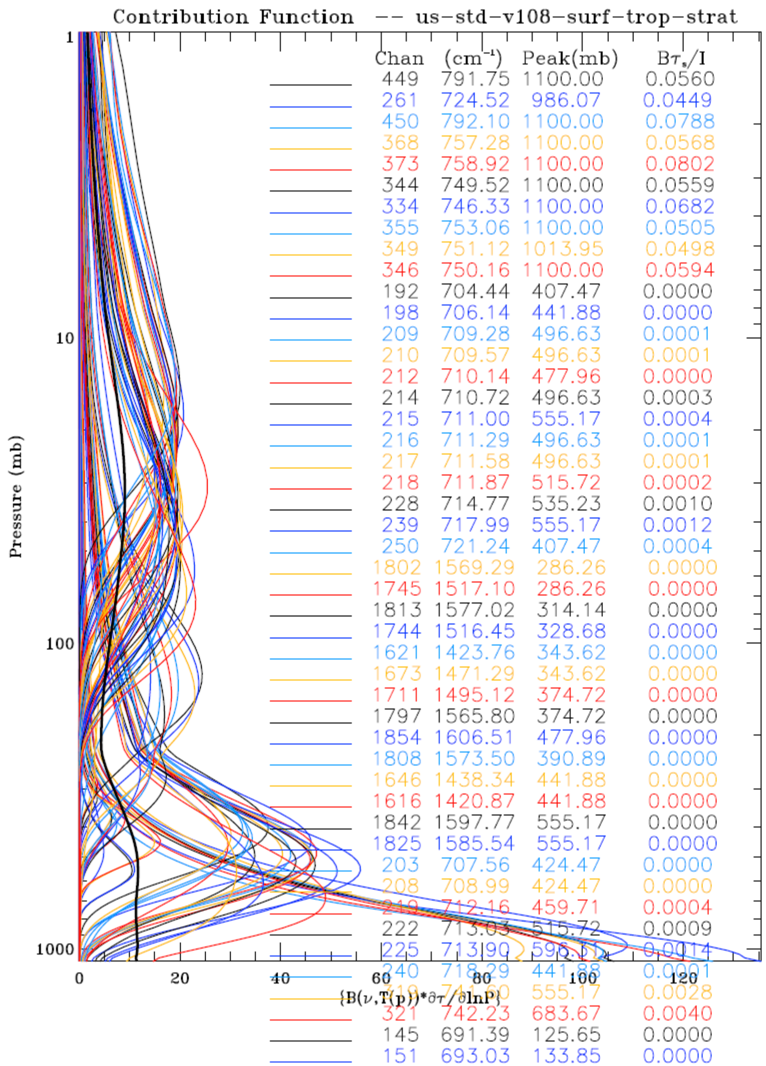
* Software framework for UQ by Sandia NLs.

AIRS profile-analysis tool



- **Definitions:**
  - TOA: Top of atmosphere
  - SARTA: Standalone AIRS Radiative-Transfer Algorithm
- **Solution for $n_{\max}=100$ vertical ($\ln p$) layers**
- **In minimizing cost functions for data retrieval, iterations allow the i^{th} input vertical profile, $x_i(\ln p)$, to be perturbed by a factor $(1+\alpha_i)$**
  - At present, the α_i are assumed uniform in altitude ($\ln p$).
  - $i = T, q, O_3$, *and* CO_2

CO_2 channel contribution functions



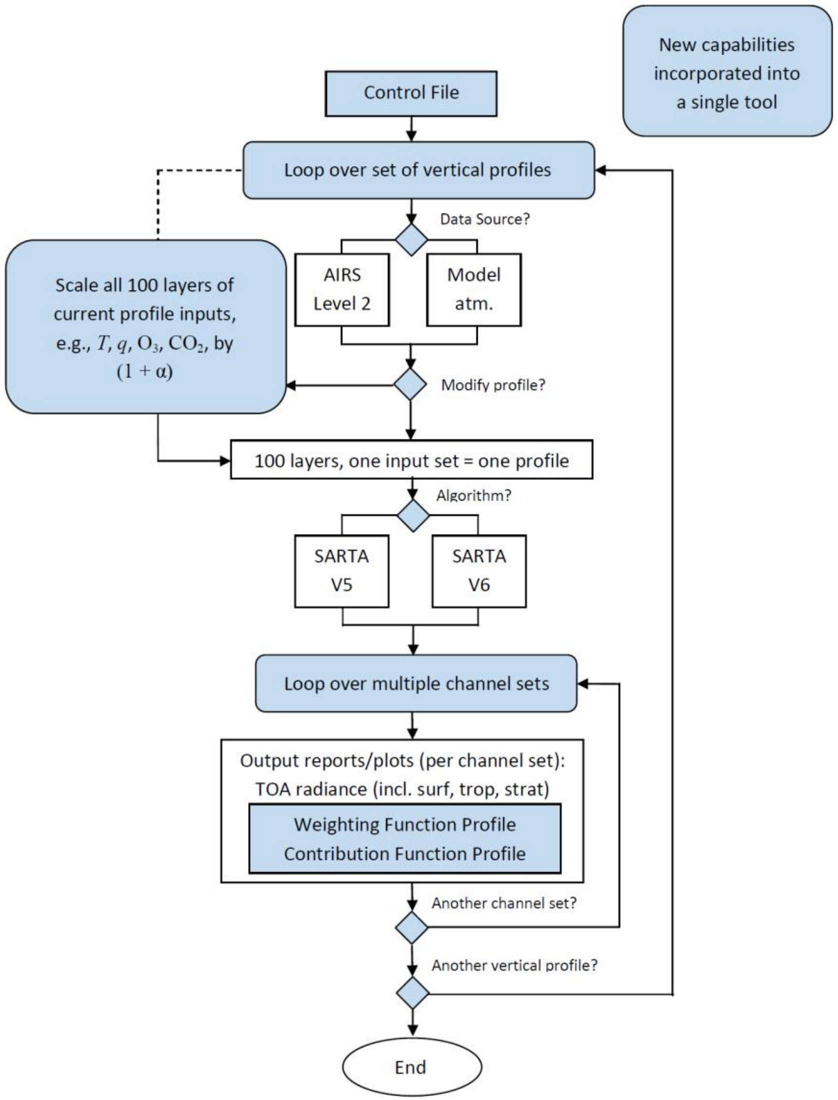
- **Radiance intensity***

$$I_\nu = \underbrace{S(\nu, T_0, \varepsilon_\nu)}_{\text{Surface contribution}} - \underbrace{\int_0^{p_0} B[\nu, T(p)] \overbrace{\frac{\partial \tau(\nu, p, \ldots)}{\partial p}}^{\text{Weighting function (WF)}}}\,\mathrm{d}p$$

- **Contribution function (CF)**
- **CF plots of channels previously identified as relevant for CO_2 retrievals in the**
  - **stratosphere,**
  - **troposphere, and**
  - **near-surface**
- **Plots estimated for U.S. std. atm.**
  - **Real atmosphere varies with place and time (location, altitude, weather, season, composition, etc.)**

* Chahine *et al*. (2005 *GRL*).

AIRS weighting-/contribution-function tool



- **Definitions:**
  - **TOA: Top of atmosphere**
  - **SARTA: Standalone AIRS Radiative-Transfer Algorithm**
- **For each channel, the tool estimates the layer profiles for the**
  - **weighting function (WF)**
  - **contribution function (CF)**
- **Scales all profiles using uniform $(1+\alpha_i)$ scaling factors from the AIRS profile-analysis tool**
  - **Solution for $n_{\max}$=100 vertical $(\ln p)$ layers**

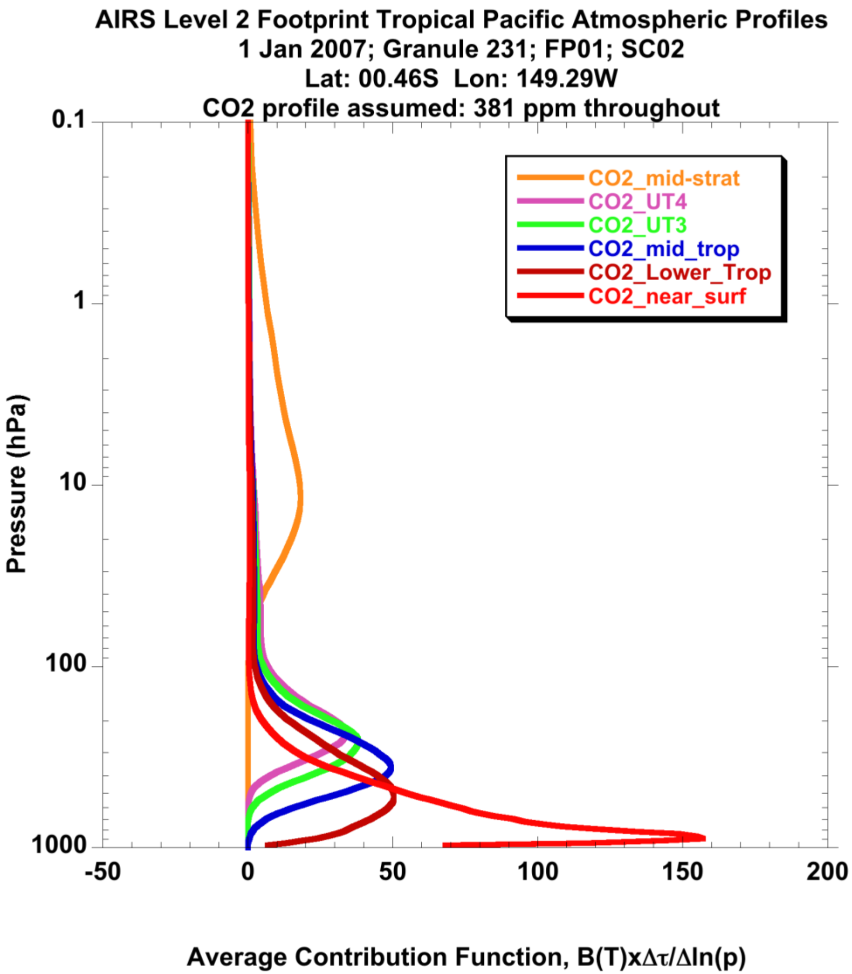
Updated retrieval-tool capabilities (at present)

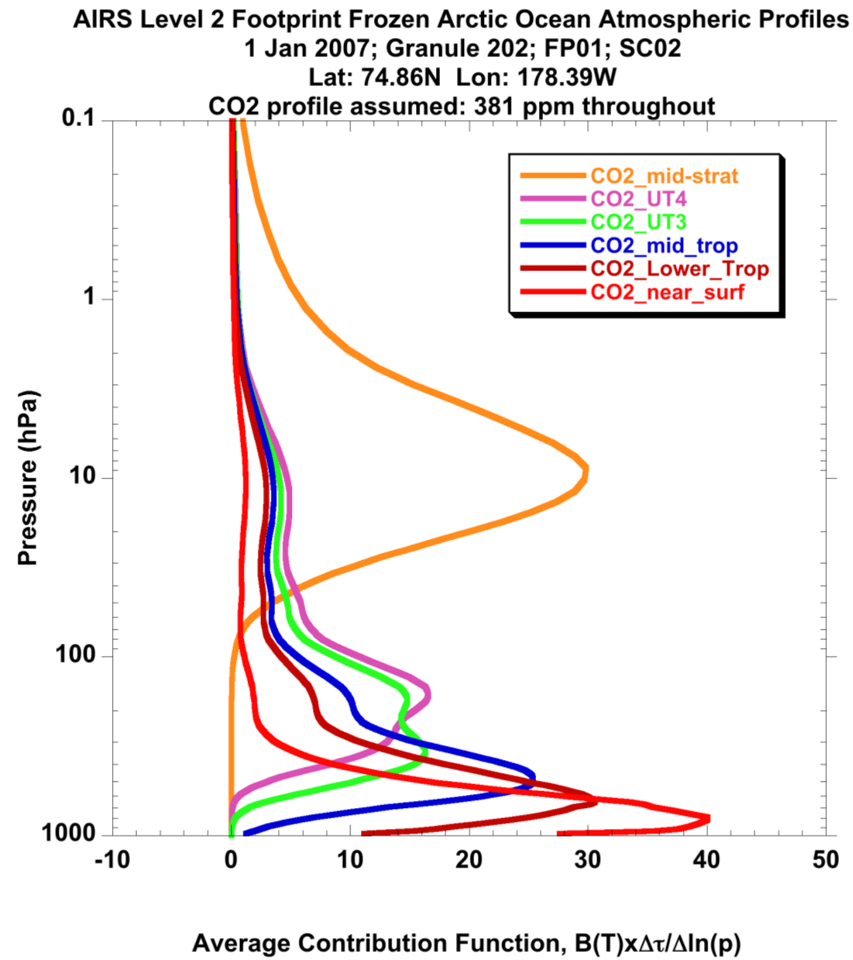
- Can ingest vertical columns of properties/constituents (T_{air}, H_2O, O_3, CO_2, and others) to SARTA and can compute:
  - Top-of-atmosphere (TOA) radiance for the AIRS 2378 IR channel set, including contributions from surface, troposphere, and stratosphere.
  - Weighting function (WF): layer-wise calculation of $d\tau(\nu, \ln p, \ldots)/d\ln(p)$
  - Contribution function (CF): $B[\nu, T(p)]\, d\tau(\nu, \ln p, \ldots)/d\ln(p)$, net TOA radiance,
    - per channel k,
    - per level n,
    - for a given temperature profile, $T_{air}(p)$
  - Analysis tools to support processing of multiple permutations of a single profile
  - Custom software wrappers to enable running retrieval tools for SA/UQ
- Enable perturbation of vertical constituent column inputs by fixed scale factors, $\alpha_i(p)$, simultaneously for all levels
  - Perturbation, layer-by-layer, and collation of changes in radiance, in response to changes in inputs, to support Jacobian/SA studies

National Aeronautics and Space Administration

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

Examples of CF aggregates for CO_2





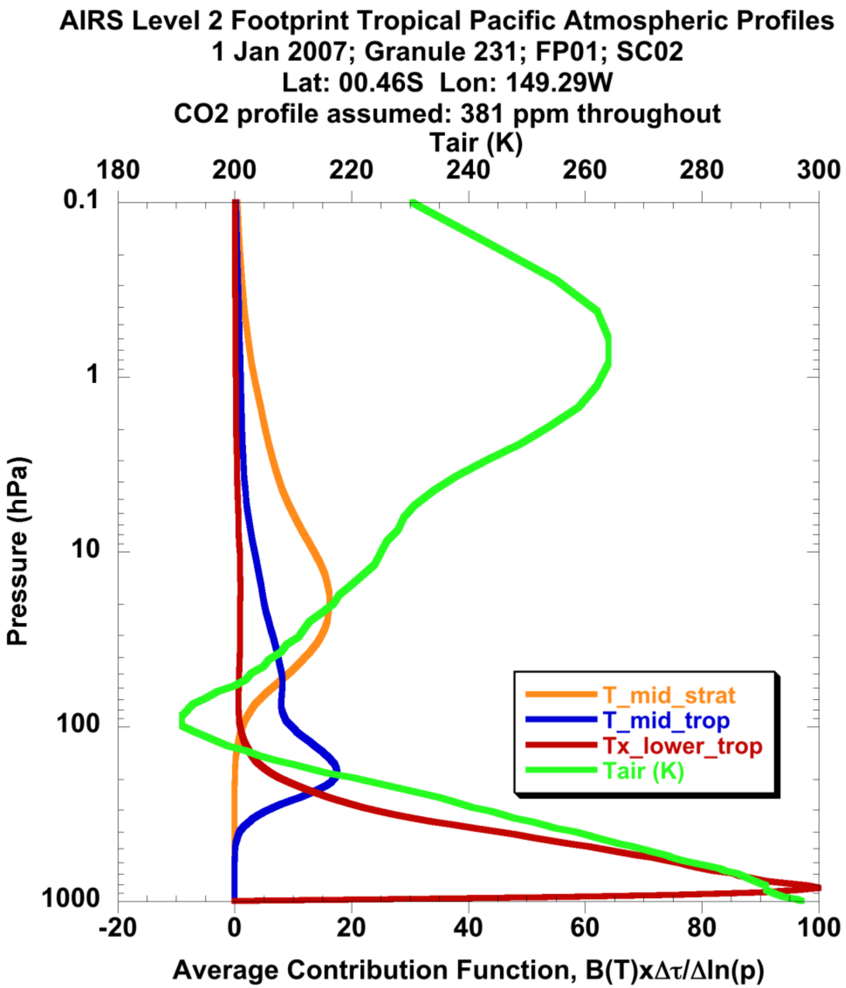
- Sufficient variance between CFs with respect to p to allow CO_2 (and other) vertical-profile estimations

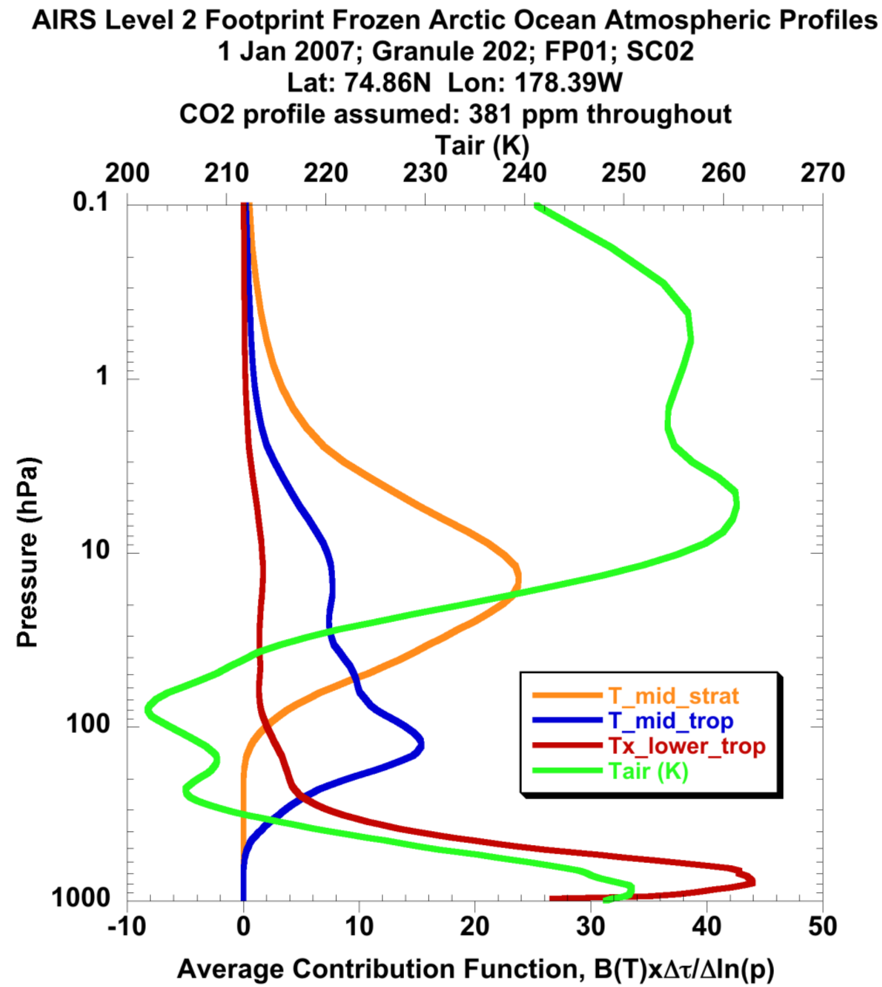
Dimotakis *et al*. 2012 Profiles with SA/UQ. *AIRS STM*

National Aeronautics and
Space Administration

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

Select CF aggregates with *T* profiles





- **Present algorithms/tools allow for small, but uniform, multiplicative shifts $(1+\alpha_i)$ for i^{th} profile: adequate for retrievals over narrow p ranges.**

Maximum Likelihood Estimation (MLE) with UQ
Simple example

TOA radiances calculation (SARTA output)

$$\theta_{\nu_m} = \theta_{\nu_m}(x_T, x_q, x_{\mathrm{O3}}, \cdots, x_{\mathrm{CO2}});\ \ x_i = x_i(n), n = 1,\ldots, n_{\max} = 100, \text{is the } i^{\text{th}} \text{ variable column vector}$$

Maximize conditional probability*

$$p(x_{\mathrm{CO2}} \mid \theta_{\nu_1}^{\mathrm{obs}}, \theta_{\nu_2}^{\mathrm{obs}}, \cdots, \theta_{\nu_M}^{\mathrm{obs}}; x_T^{\mathrm{b}}, x_q^{\mathrm{b}}, x_{\mathrm{O3}}^{\mathrm{b}}, x_{\mathrm{CO2}}^{\mathrm{b}}, \ldots)$$

Minimize the cost function (varying x_{CO2} only)

$$J(x_{\mathrm{CO2}}) = \frac{1}{2}\sum_{m=1}^{M}\left[\theta_{\nu_m}^{\mathrm{obs}} - \theta_{\nu_m}\left(x_T^{\mathrm{b}}, x_q^{\mathrm{b}}, x_{\mathrm{O3}}^{\mathrm{b}}, x_{\mathrm{CO2}}\right)\right]^{\mathrm{T}} R_{\nu_m\nu_m}^{-1}\left[\theta_{\nu_m}^{\mathrm{obs}} - \theta_{\nu_m}\left(x_T^{\mathrm{b}}, x_q^{\mathrm{b}}, x_{\mathrm{O3}}^{\mathrm{b}}, x_{\mathrm{CO2}}\right)\right]$$
$$+\frac{1}{2}\left(x_{\mathrm{CO2}} - x_{\mathrm{CO2}}^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}_{\mathrm{CO2}}^{-1}\left(x_{\mathrm{CO2}} - x_{\mathrm{CO2}}^{\mathrm{b}}\right)$$

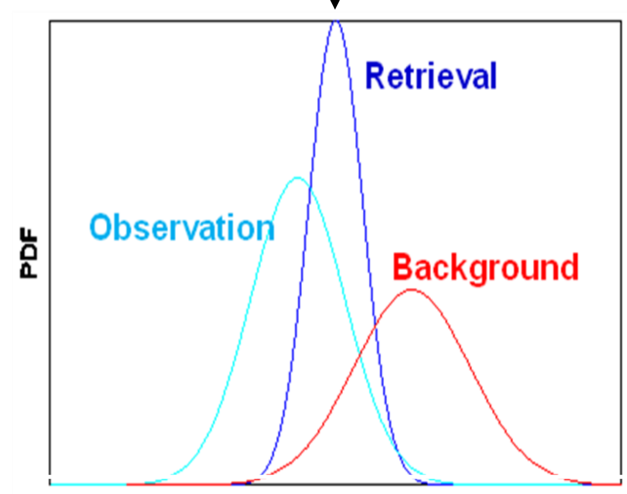
Retrieved $\mathrm{CO_2}$ error covariance

$$\mathbf{P}_{\mathrm{CO2}} = (\mathbf{B}^{-1} + \mathbf{H}_{\mathrm{CO2}}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}_{\mathrm{CO2}})^{-1}$$
$$= \mathbf{B} - \mathbf{B}\mathbf{H}_{\mathrm{CO2}}^{\mathrm{T}}\left(\mathbf{H}_{\mathrm{CO2}}\mathbf{B}\mathbf{H}_{\mathrm{CO2}}^{\mathrm{T}} + \mathbf{R}\right)^{-1}\mathbf{H}_{\mathrm{CO2}}\mathbf{B}$$

B*:* Background-error covariance

R*:* Observational-error covariance

$\mathbf{H}_{\mathrm{CO2}}$: Jacobian, sensitivity matrix

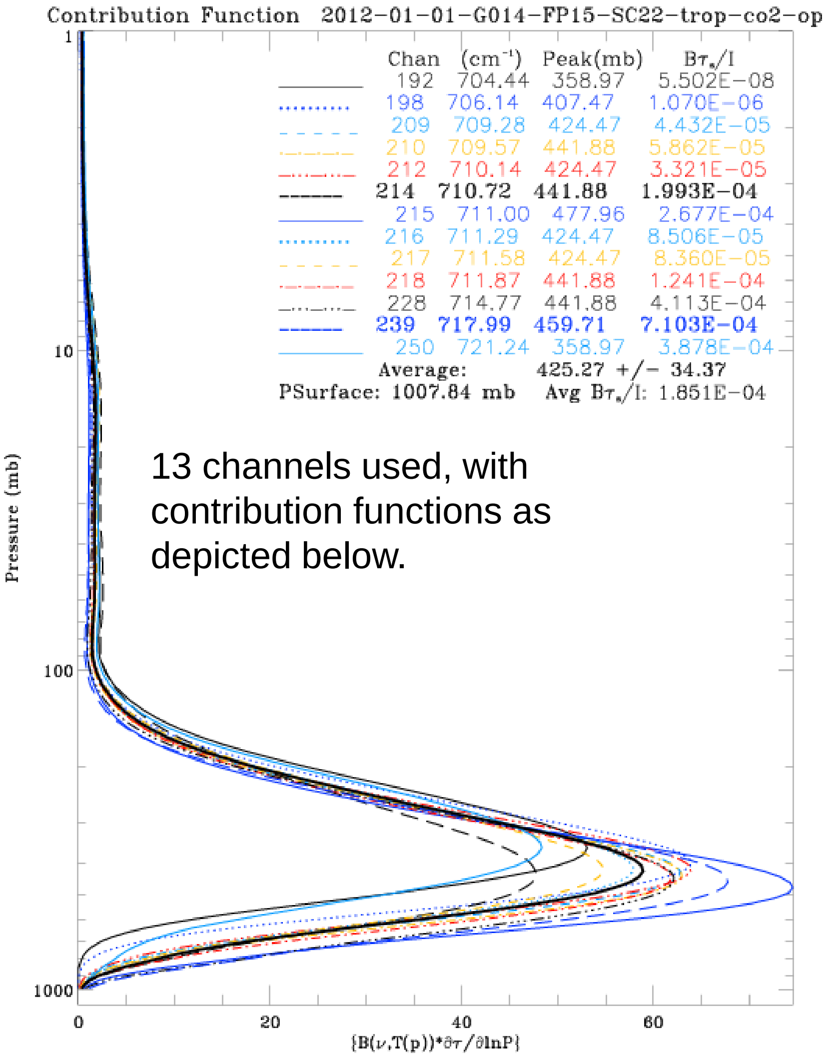


Maximum-Likelihood Estimate

* Superscripts: "obs"=observation/measurement, "b"=background/priors

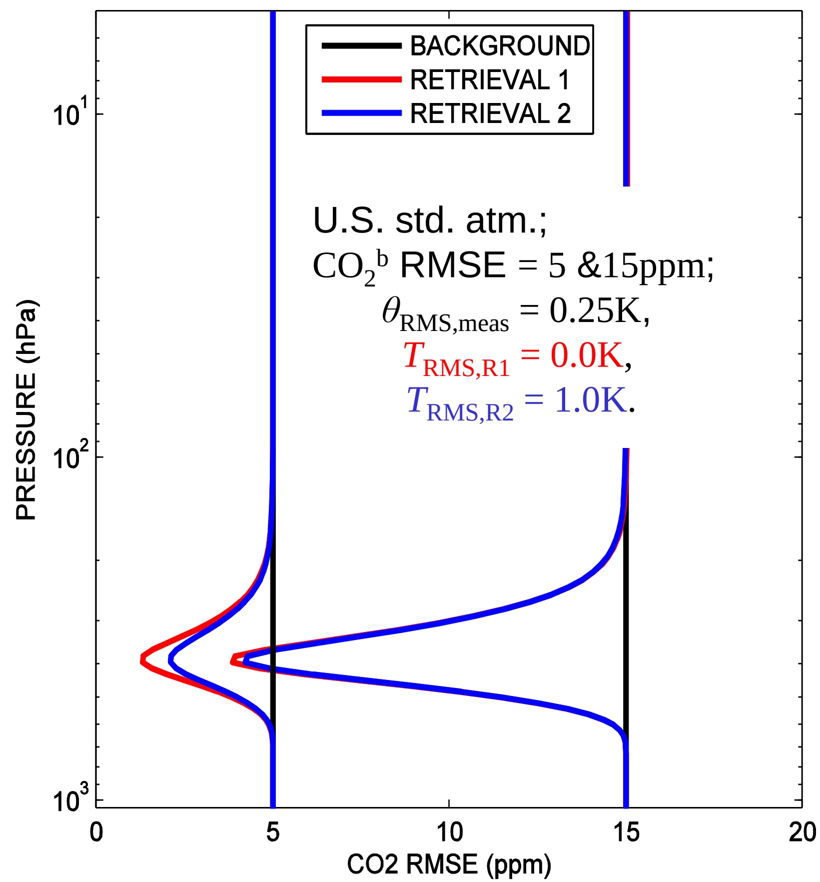
Dimotakis *et al*. 2012 Profiles with SA/UQ. *AIRS STM*

A simple illustration of retrieved CO_2 RMSE



13 channels used, with contribution functions as depicted below.

Dependence of retrieved CO_2 RMSE on background T and CO_2 (priors) RMSE.



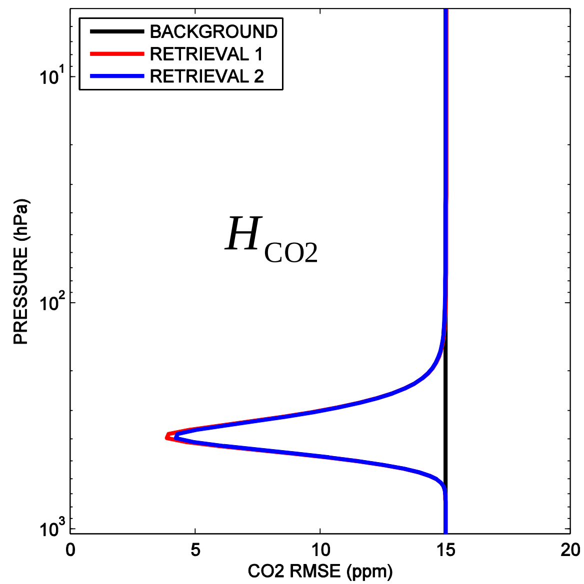
Dimotakis *et al*. 2012 Profiles with SA/UQ. *AIRS STM*

Channel brightness temperatures and their sensitivity to CO_2, and retrieved CO_2 RMSE

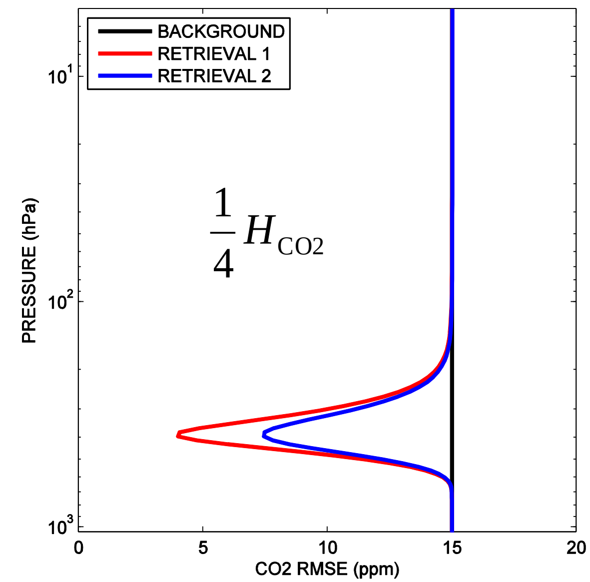
Jacobian/sensitivity*

$$H_{\mathrm{CO2}} = \left[\frac{\partial\theta_{\nu_1}\left(x_T^{\mathrm{b}}, x_q^{\mathrm{b}}, x_{\mathrm{O3}}^{\mathrm{b}}, x_{\mathrm{CO2}}^{\mathrm{b}}\right)}{\partial x_{\mathrm{CO2}}^{\mathrm{t}}}, \frac{\partial\theta_{\nu_2}\left(x_T^{\mathrm{b}}, x_q^{\mathrm{b}}, x_{\mathrm{O3}}^{\mathrm{b}}, x_{\mathrm{CO2}}^{\mathrm{b}}\right)}{\partial x_{\mathrm{CO2}}^{\mathrm{t}}}, \cdots, \frac{\partial\theta_{\nu_M}\left(x_T^{\mathrm{b}}, x_q^{\mathrm{b}}, x_{\mathrm{O3}}^{\mathrm{b}}, x_{\mathrm{CO2}}^{\mathrm{b}}\right)}{\partial x_{\mathrm{CO2}}^{\mathrm{t}}}\right]$$

High sensitivities



Lower sensitivities



Importance of high sensitivities ➡

1. **Lower retrieval RMSE**
2. **Less-sensitive to errors in other parameters**
3. **Channel selection and retrieval algorithms**

Dimotakis *et al*. 2012 Profiles with SA/UQ. *AIRS STM*

* Superscripts: “b” = background/priors; “t” = true value

Future plans

- **Further extend and generalize SARTA use**
  - **Support systematic, large-scale sensitivity analyses (SA)**
  - **Allow for p-dependent input scaling functions, $\alpha_i(\ln p)$.**
  - **Explore and support Monte Carlo techniques and DAKOTA for retrieval UQ**
- **Perform UQ on multi-season mid-tropospheric retrievals**
  - **Compare with V5 retrievals**
  - **Explore relation and application to V6 retrievals**
- **Extend SA/UQ concepts and formulations and assess their applicability to the retrieval of vertical profiles for:**
  - **stratospheric layers,**
  - **low-troposphere, and**
  - **near-surface retrievals.**
- **Explore functional-projection analyses for vertical-profile estimation**
- **Apply to instrument calibration, enhance algorithm verification, and use available data for quantitative validation**

Thank you.